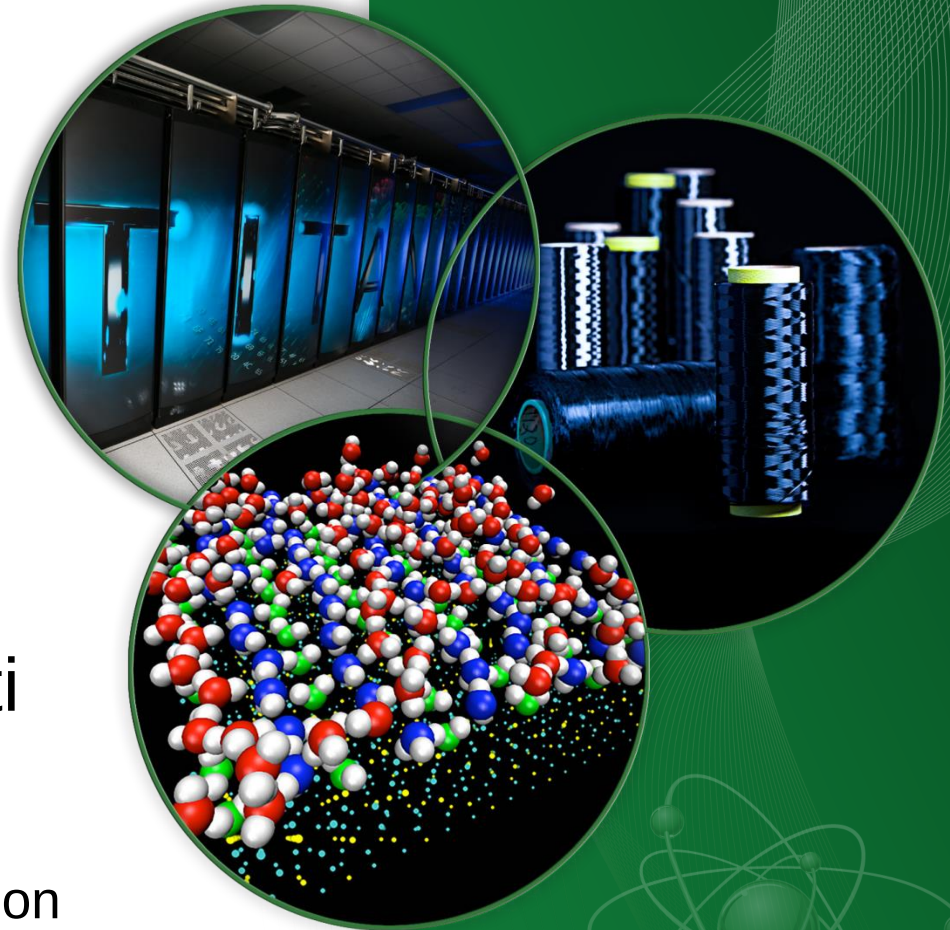
Development and Testing of Advanced S/U Methods for NCS Analyses



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Introduction

- Sensitivity coefficients describe the change in a system response that occurs due to uncertainty or perturbations in system parameters.

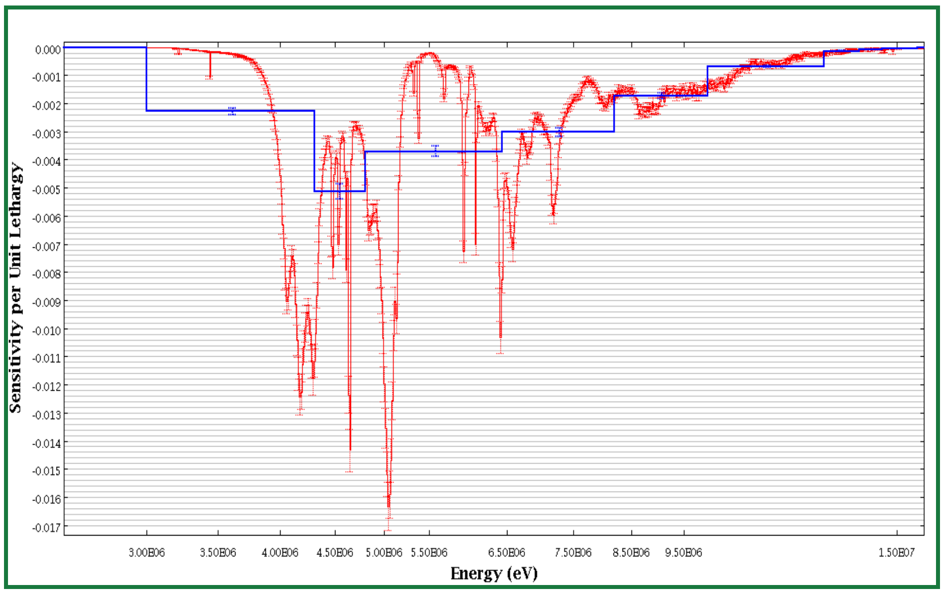
$$S_{R,\Sigma_x} = \frac{\delta R/R}{\delta \Sigma_x/\Sigma_x}$$

- The SCALE code contains a suite of eigenvalue (k_{eff}) sensitivity and uncertainty analysis tools using the TSUNAMI code, which has proven indispensable for numerous application and design studies for nuclear criticality safety and reactor physics.

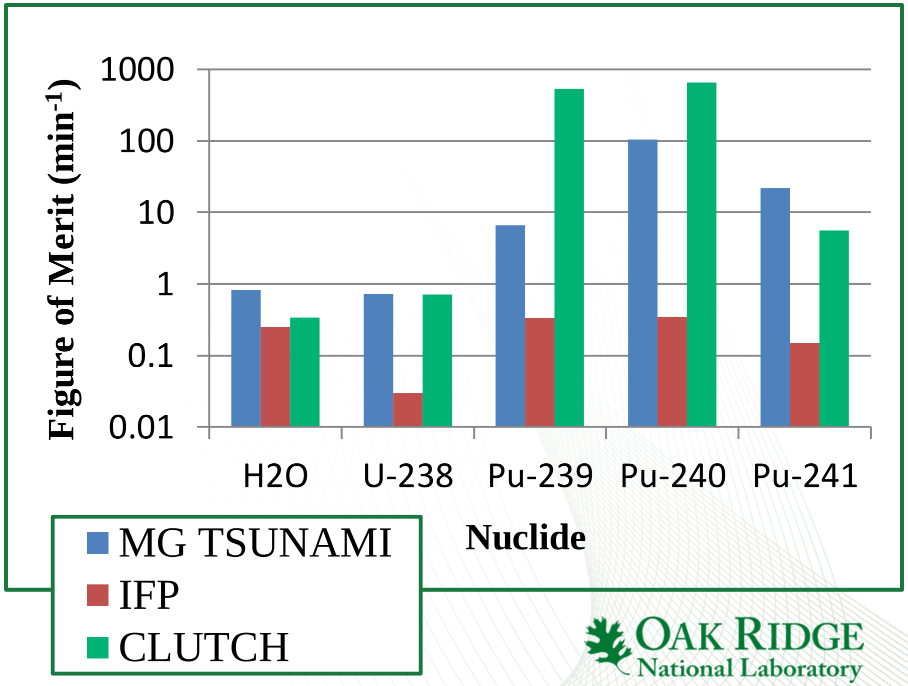
Introduction: Previous Work

- Recent NCSP-supported work has enabled the traditionally multigroup TSUNAMI-3D code to be extended to continuous-energy applications.
  - This work involved the development of the CLUTCH sensitivity method, a new and efficient approach for calculating eigenvalue sensitivity coefficients.

O-16 Capture Sensitivity
238-group VS
Microgroup CLUTCH



MIX-COMP-THERM-004-001
FoM Comparison



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Introduction

- This work has extended the Continuous-Energy (CE) TSUNAMI-3D eigenvalue sensitivity coefficient capabilities to enable a first-ever approach for calculating sensitivity coefficients for generalized neutronic responses in 3D, CE Monte Carlo simulations.
  - This was accomplished by combining the two approaches in CE TSUNAMI-3D for calculating eigenvalue sensitivity coefficients: the CLUTCH and Iterated Fission Probability (IFP) methods.
- This new generalized response sensitivity capability has been named the GEneralized Adjoint Responses in Monte Carlo (GEAR-MC) Method.

Generalized Perturbation Theory

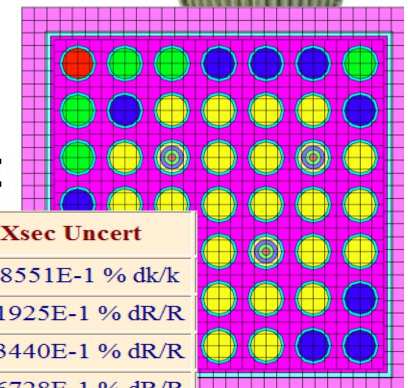
- Generalized Perturbation Theory (GPT) estimates sensitivity coefficients for any system response that can be expressed as the ratio of reaction rates.

$$R = \frac{\langle \Sigma_1 \phi \rangle}{\langle \Sigma_2 \phi \rangle}$$

- Calculating generalized sensitivity coefficients requires solving an inhomogeneous, or generalized, adjoint equation:

$$L^{\dagger} \Gamma^{\dagger} = \lambda P^{\dagger} \Gamma^{\dagger} + S^{\dagger}$$

$$S^{\dagger} = \frac{1}{R}\frac{\partial R}{\partial \phi} = \frac{\Sigma_1}{\langle \Sigma_1 \phi \rangle} - \frac{\Sigma_2}{\langle \Sigma_2 \phi \rangle}$$



- Applications for GPT sensitivity/uncertainty analysis include:
  - Relative Powers
  - Isotope Conversion Ratios
  - Multigroup Cross Sections
  - Experimental Parameters

NUMBER	EXPERIMENT	Type	Format	Value	Xsec Uncert
1	k_infinity	keff	Relative	1.1083E+0	4.98551E-1 % dk/k
2	fission_grp_1	gpt	Relative	1.9155E-3	6.91925E-1 % dR/R
3	fission_grp_2	gpt	Relative	2.7748E-2	3.23440E-1 % dR/R
4	absorpt_grp_1	gpt	Relative	7.1637E-3	8.36728E-1 % dR/R
5	absorpt_grp_2	gpt	Relative	5.3702E-2	2.38082E-1 % dR/R
6	cornerrod_fpf	gpt	Relative	1.1458E+0	1.67147E-1 % dR/R

OECD UAM GPT Benchmark Phase 1-2 Results

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Theory

- The generalized importance function for a response can be expressed as the sum of two terms: the intra-generation effect term and the inter-generational effect term.
  - The **intra-generation** effect describes how much importance a neutron generates after an event occurs.
  - The **inter-generational** effect describes the importance that is generated by the daughter fission neutrons of the original particle.

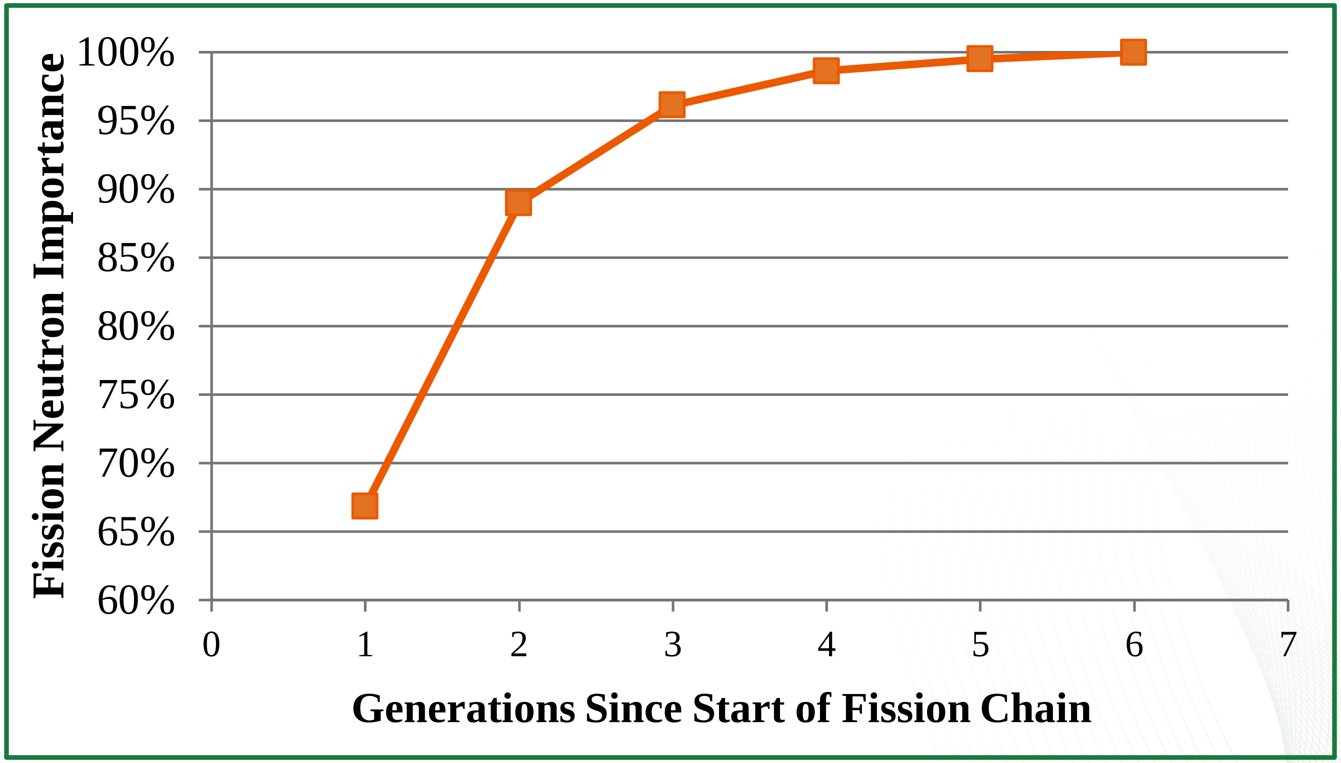
$$\Gamma^{\dagger}(\tau_s) = \boxed{\frac{1}{Q_s}\langle\frac{1}{R}\frac{\partial R}{\partial \phi}(r)\phi(\tau_s \to r)\rangle} + \boxed{\frac{\lambda}{Q_s}\langle\Gamma^{\dagger}(r)P(r)\phi(\tau_s \to r)\rangle}$$

- The **CLUTCH** sensitivity method is used to calculate the intra-generation term, and an Iterated Fission Probability-based approach calculates the inter-generational term.

- $\frac{1}{R}\frac{\partial R}{\partial \phi}(r)$ contains both positive and negative terms. Thus, events during a particle history can generate either positive or negative importance.

Inter-generational Importance

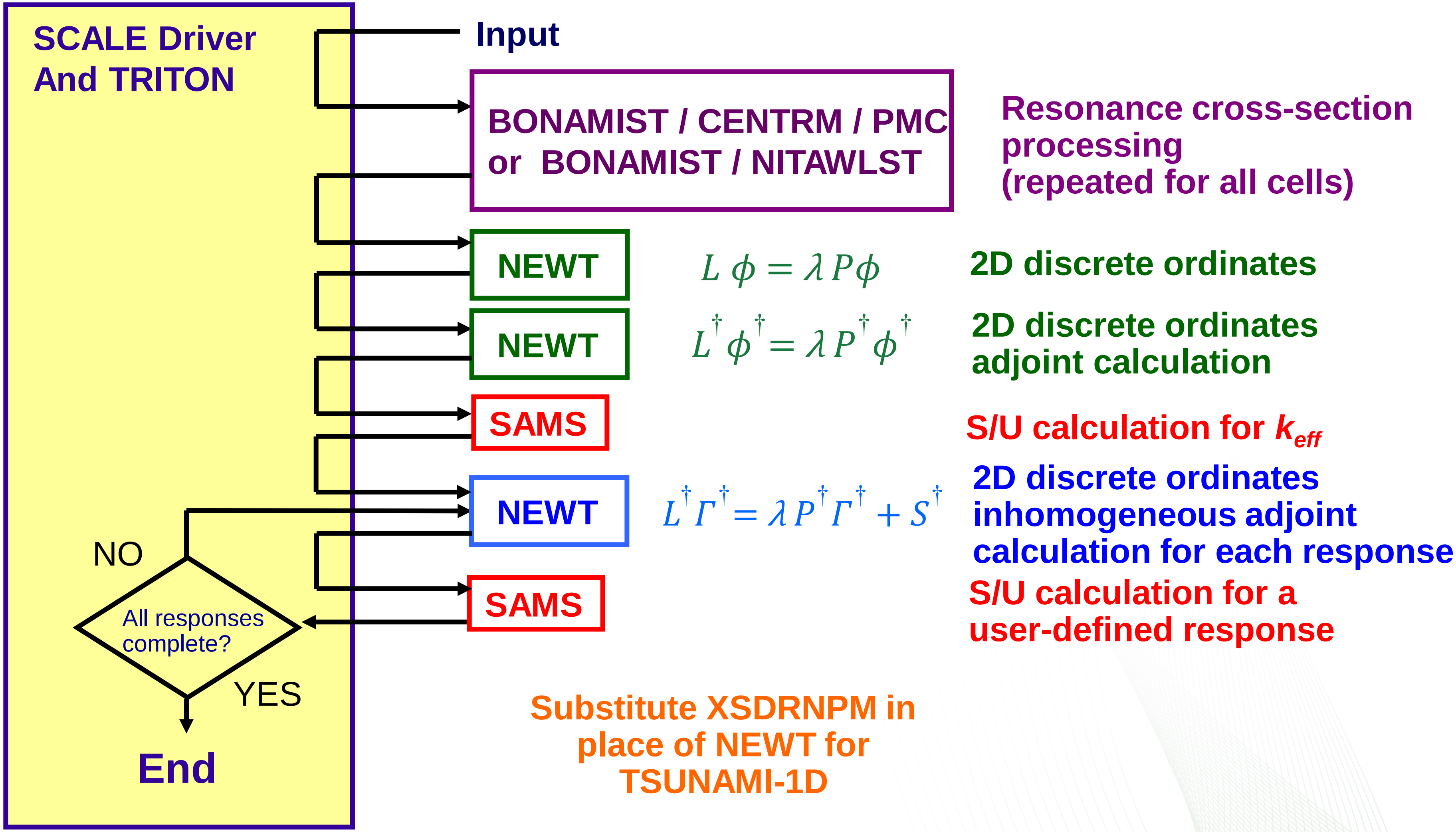
- The inter-generational term is calculated by tallying the intra-generational importance generated by neutrons in a fission chain as that importance approaches zero.
  - ➢ This term is tallied using the IFP method.



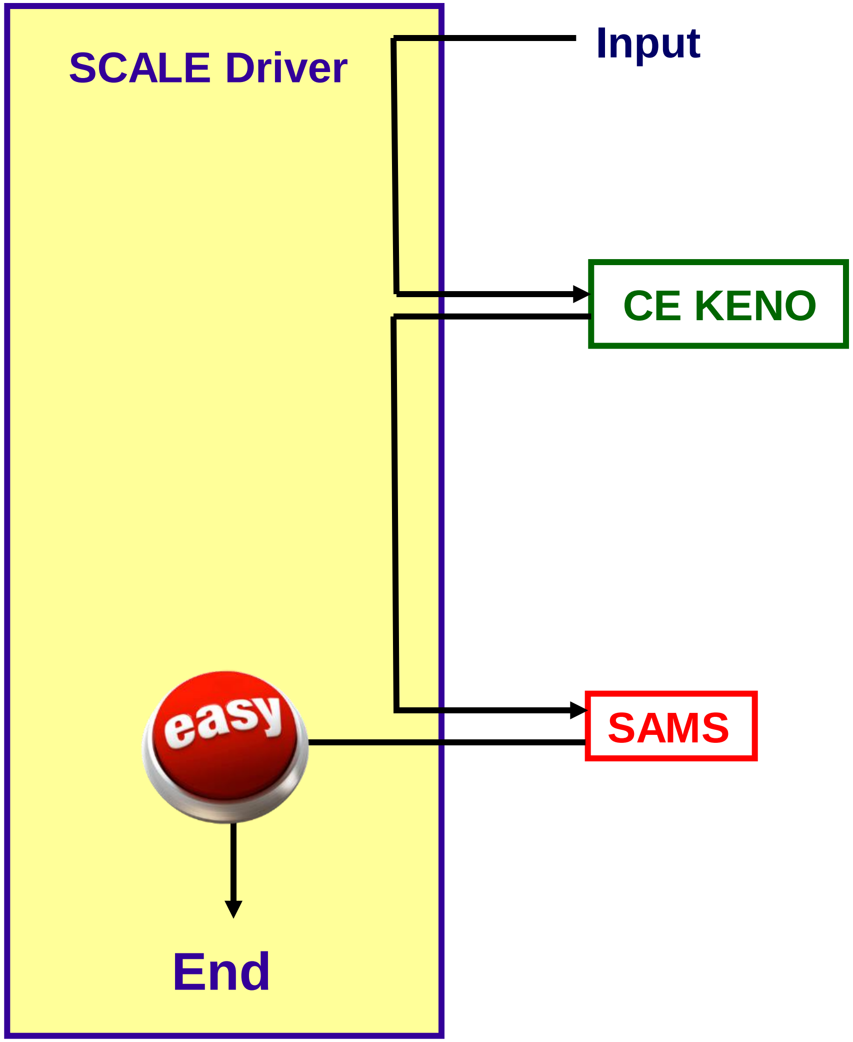
How does this approach differ from existing methods?

- Generalized Perturbation Theory Monte Carlo methods have been developed by Abdel-Khalik et al. for calculating generalized sensitivity coefficients in 3D, continuous-energy Monte Carlo applications, but these methods require performing multiple direct perturbation calculations and can require a large number of runs to calculate generalized sensitivity coefficients.
- This approach differs in that it:
  - Requires no perturbation calculations and no knowledge of nuclear covariance data.
  - Because our approach is not perturbation-based, we can easily calculate energy-dependent sensitivity coefficients for multiple responses to all input nuclear data parameters in one continuous-energy Monte Carlo transport calculation.
  - The deterministic, sensitivity-based TSUNAMI-1D and TSUNAMI-2D GPT methods require at least one transport calculation per generalized response.

TSUNAMI-1D/2D GPT Sequences



CE TSUNAMI-3D GPT Sequence



3D Monte Carlo

$$L\,\phi = \lambda\,P\phi$$

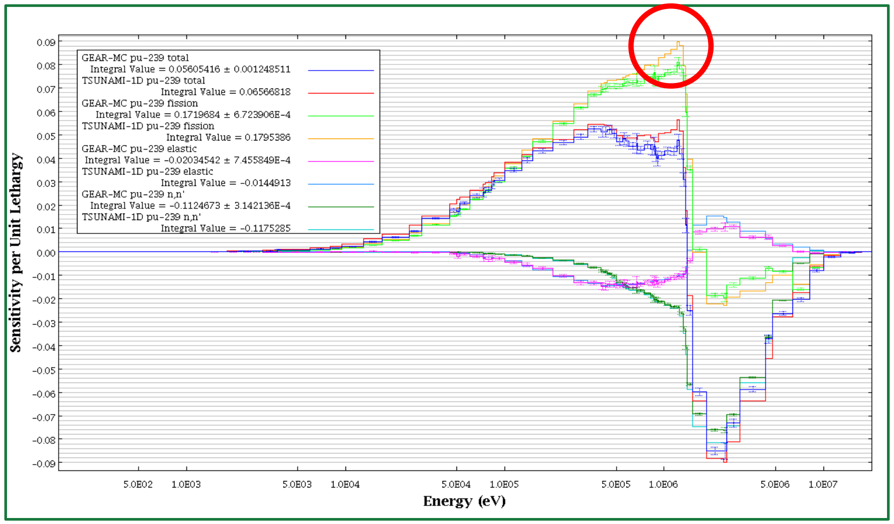
$$L^{\dagger}\phi^{\dagger} = \lambda\,P^{\dagger}\phi^{\dagger}$$

$$L^{\dagger}\Gamma^{\dagger} = \lambda\,P^{\dagger}\Gamma^{\dagger} + S^{\dagger}$$

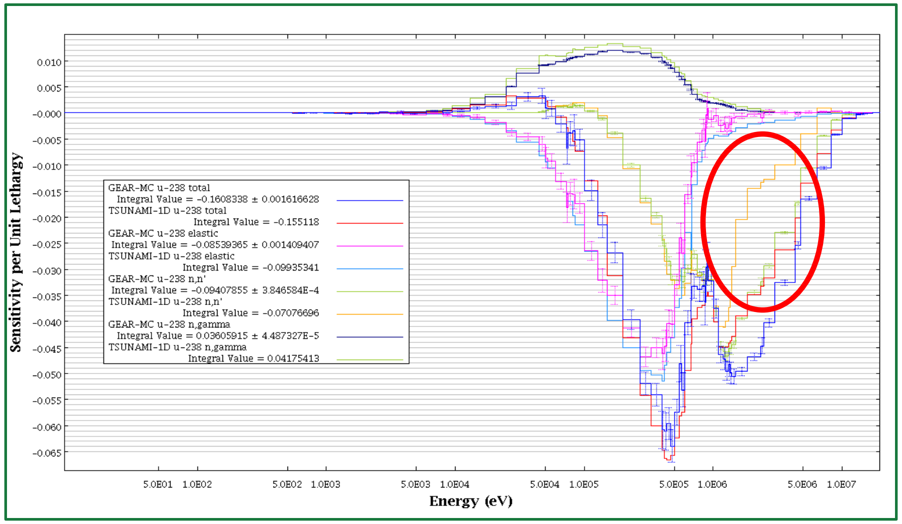
S/U calculation for k_{eff} and user-defined responses

GPT Flattop Foil Response Sensitivity Coefficients

F28/F25 Pu-239 Sensitivity Coefficients



F37/F25 U-238 Sensitivity Coefficients



Flattop Total Nuclide Foil Response Sensitivities

Experiment	Response	Isotope	Direct Pert.	TSUNAMI-1D	GEAR-MC
Flattop	F28 / F25	U-238	0.8006 ± 0.0533	0.8024 **(0.03 σ)**	0.7954 ± 0.0018 **(-0.10 σ)**
		Pu-239	0.0528 ± 0.0043	0.0657 **(2.99 σ)**	0.0561 ± 0.0012 **(0.73 σ)**
	F37 / F25	U-238	-0.1540 ± 0.0102	-0.1551 **(-0.11 σ)**	-0.1608 ± 0.0016 **(-0.66 σ)**
		Pu-239	0.0543 ± 0.0048	0.0736 **(3.99 σ)**	0.0489 ± 0.0010 **(-1.10 σ)**

Part Two:

GEAR-MC Efficiency Improvements

The IFP Method

- Originally a modified version of the Iterated Fission Probability (IFP) Method was used to tally the inter-generational term.
- The IFP Method can produce large memory footprints for systems with a large number of materials, isotopes, etc.

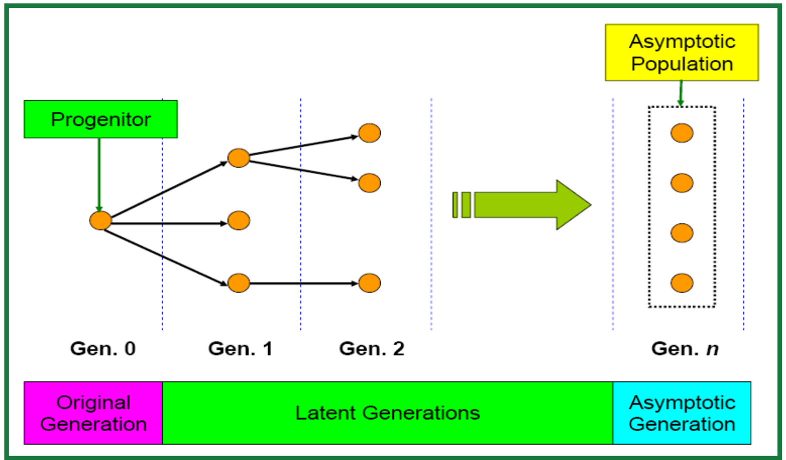
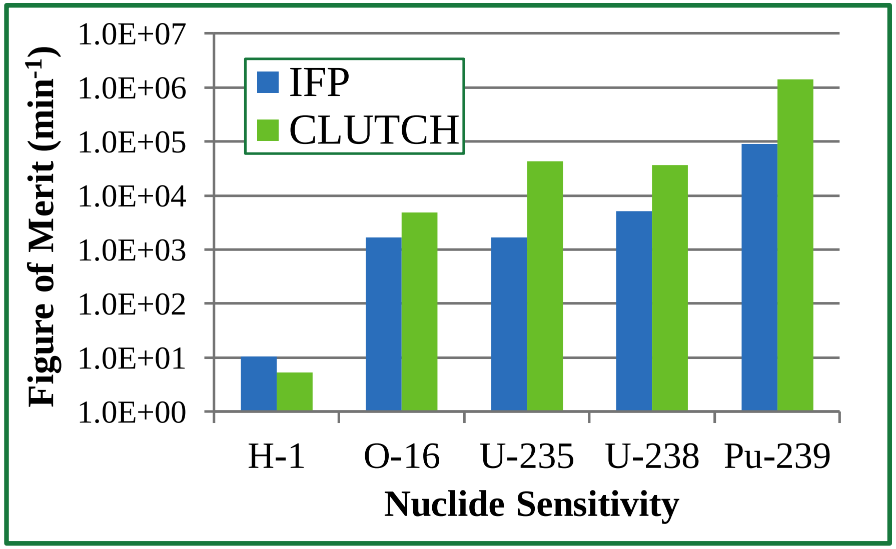


Illustration of the IFP Process.
Image courtesy of Brian Kiedrowski.



Sensitivity Method Memory Usage		
Model	**CLUTCH**	**IFP**
Fuel Pin	1.06 MB	2,113 MB
Godiva	0.12 MB	26 MB
HMF-025-005	0.16 MB	1,675 MB
LCT-010-014	25 MB	19,509 MB
NAC-UMS	3,416 MB	21,201 MB

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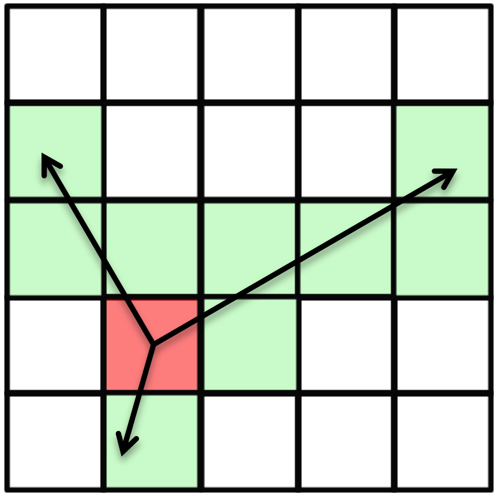
The F*(r) Function

- The CLUTCH Method uses an importance weighting function, F*(r), to compute multi-generational sensitivity effects.
- The F*(r) function describes the average response importance generated by fission neutrons born at location r.

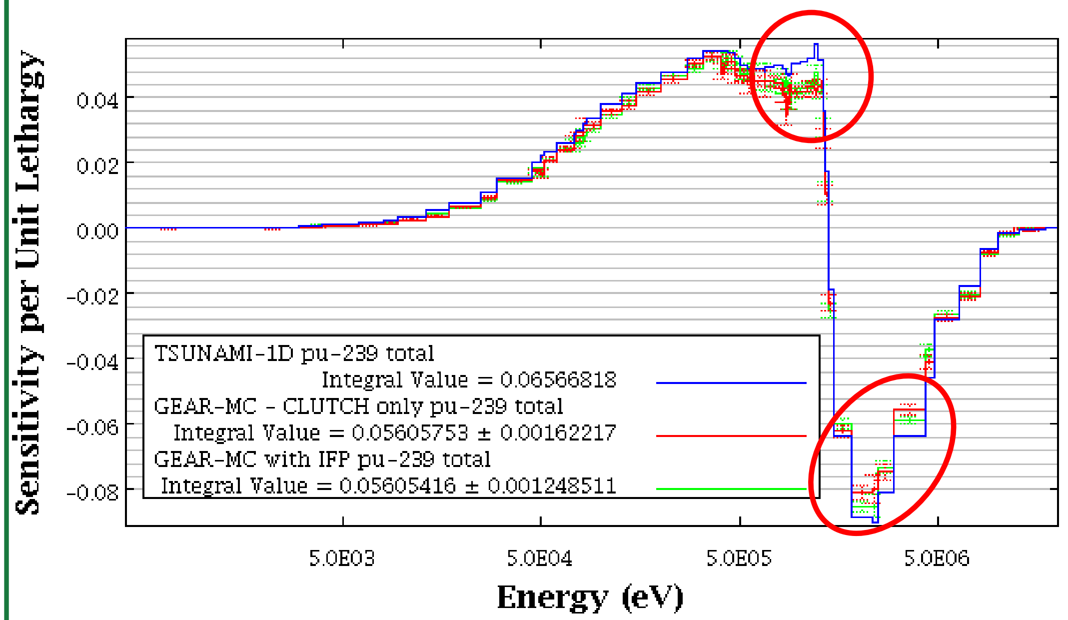


- The F*(r) function can be calculated using the IFP method during inactive generations with NO loss of accuracy and with significant memory savings.
- This work also sought to extend the concept of F*(r) to compute the inter-generational effect term in GEAR-MC GPT sensitivity calculations.

Evaluation of Accuracy: GPT Flattop Foil Response Sensitivity Coefficients

Generalized sensitivity coefficients were calculated for models of several criticality safety systems to:

- Evaluate the accuracy of the F*(r) approach.
- Explore the potential improvements in computational efficiency.



Flattop F28/F25 Pu-239 Sensitivity Coefficients

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Evaluation of Accuracy: GPT Flattop Foil Response Sensitivity Coefficients

- The CLUTCH-only GEAR-MC calculations showed good agreement with both the conventional GEAR-MC and the reference Direct Perturbation sensitivity coefficients.

Experiment	Response	Isotope	Direct Pert.	TSU-1D	GEAR-MC with IFP	GEAR-MC CLUTCH only
Flattop	F28 / F25	U-238	0.8006 ± 0.0533	0.8024 (**0.03 σ**)	0.7954 ± 0.0018 (**-0.10 σ**)	0.7870 ± 0.0040 (**-0.26 σ**)
		Pu-239	0.0528 ± 0.0043	0.0657 (**2.99 σ**)	0.0561 ± 0.0012 (**0.73 σ**)	0.0561 ± 0.0016 (**0.71 σ**)
	F37 / F25	U-238	-0.1540 ± 0.0102	-0.1551 (**-0.11 σ**)	-0.1608 ± 0.0016 (**-0.66 σ**)	-0.1634 ± 0.0040 (**-0.86 σ**)
		Pu-239	0.0543 ± 0.0048	0.0736 (**3.99 σ**)	0.0489 ± 0.0010 (**-1.10 σ**)	0.0557 ± 0.0015 (**0.27 σ**)

Memory Usage

- Moving away from an IFP-based approach resulted in significant reductions in the computational memory footprint of simulations.

GEAR-MC Memory Usage

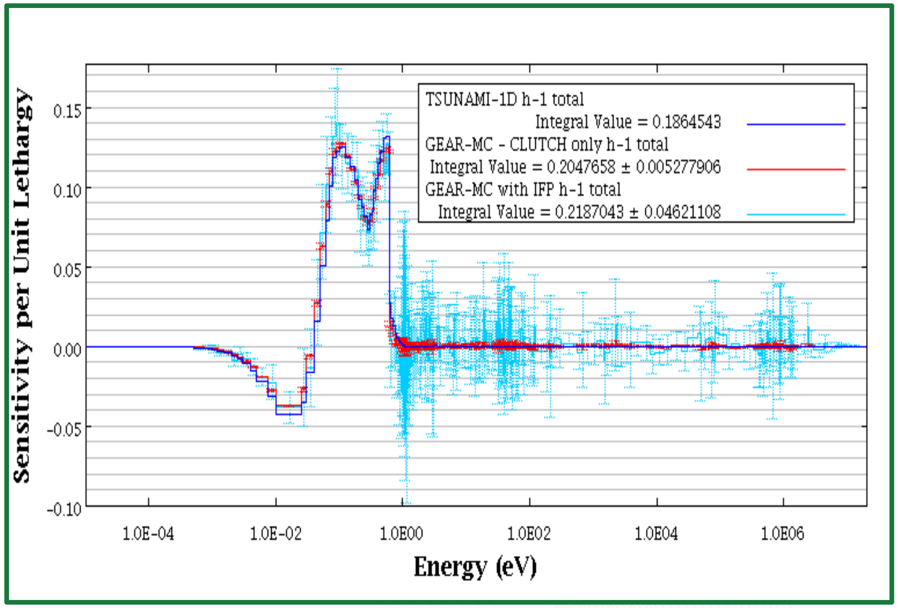
Model	GEAR-MC with IFP	GEAR-MC CLUTCH only	Memory Reduction
Godiva	581 MB	2.8 MB	99.52%
Flattop	1,082 MB	5.2 MB	99.52%
Fuel Pin	6,358 MB	3.2 MB	99.95%

Computational Efficiency

- Moving to a CLUTCH-only approach resulting in significantly improved computational efficiency for several cases.
- The Flattop calculations experienced an unexpected drop in efficiency when using an F*(r) mesh.

GEAR-MC Performance Metrics

Model	Average Runtime (hours)		Average Speedup
	IFP	CLUTCH	
Godiva	328.2	165.3	26.0
Flattop	261.1	197.1	0.52
Fuel Pin	191.4	44.1	10.25

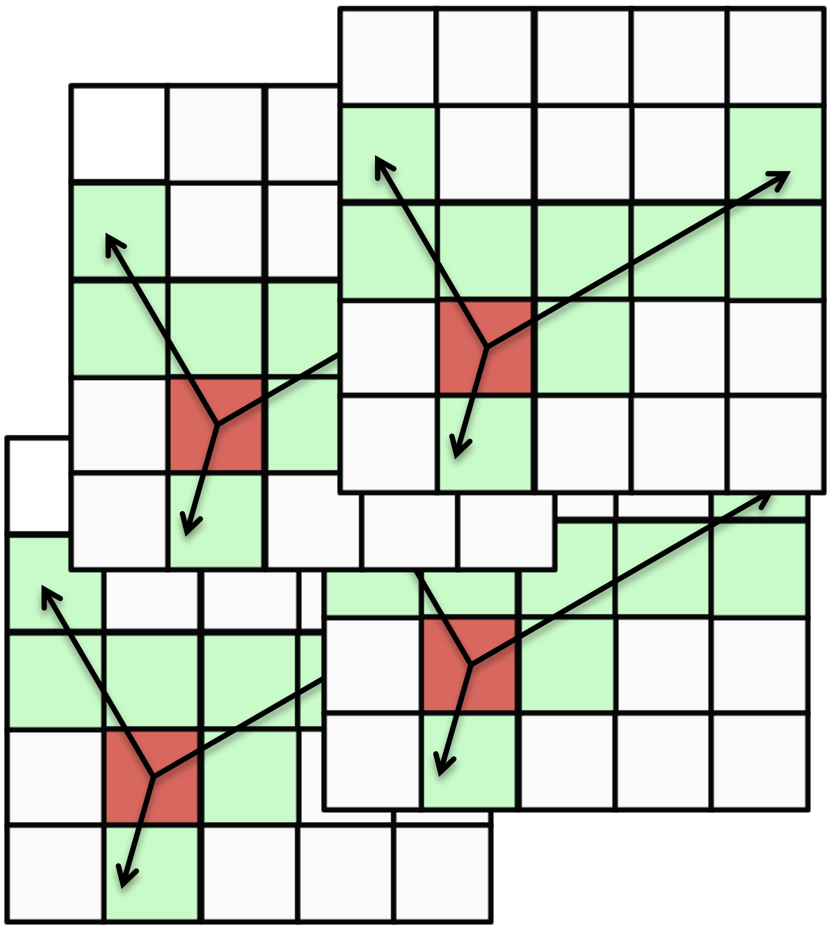


Fuel Pin Thermal Fission Cross-Section Sensitivity to H-1

Scaling and Memory Usage

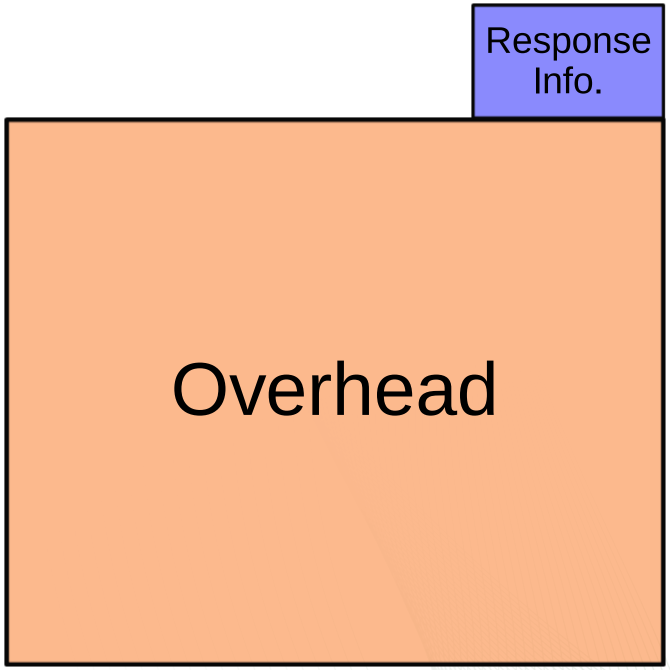
CLUTCH

One F*(r) Mesh per Response



IFP

Large Initial Overhead, Low Additional Memory per Response



Conclusions and Future Work

- The recently developed GEAR-MC method presents a first-of-its-kind approach for calculating sensitivity coefficients for generalized neutronic responses using continuous-energy, 3D Monte Carlo methods.
- The F*(r) mesh approach, which was originally developed for CLUTCH eigenvalue sensitivity calculations, was successfully extended to GEAR-MC GPT calculations.
- Removing the need to perform IFP calculations significantly reduced the memory footprint and, in some instances, improved the efficiency of the sensitivity calculations.
- The best approach for GEAR-MC calculations is likely problem-dependent, and F*(r) meshes in systems that are physically large, require a finely-resolved mesh, or contain a large number of responses may create significant memory footprints.

Questions???

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